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MICROMECHANICS OF HIERARCHICAL MATERIALS: A BRIEF OVERVIEW

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Abstract. A short overview of micromechanical models of hierarchical materials (hybrid composites, biomaterials, fractal materials, *etc*.) is given. Several examples of the modeling of strength and damage in hierarchical materials are summarized, among them, 3D FE model of hybrid composites with nanoengineered matrix, fiber bundle model of UD composites with hierarchically clustered fibers and 3D multilevel model of wood considered as a gradient, cellular material with layered composite cell walls. The main areas of research in micromechanics of hierarchical materials are identified, among them, the investigations of the effects of load redistribution between reinforcing elements at different scale levels, of the possibilities to control different material properties and to ensure synergy of strengthening effects at different scale levels and using the nanoreinforcement effects. The main future directions of the mechanics of hierarchical materials are listed, among them, the development of “concurrent” modeling techniques for hierarchical materials, optimal microstructure design at multiple scale levels using synergy effects, and the mechanical modeling of atomistic effects.

1. INTRODUCTION

Hierarchical, multiscale composites and methods of their modeling attract a growing interest of the scientific community. This interest was initially stimulated by investigations of biomaterials (wood, bones, *etc*.), which suggested that the hierarchical architectures of the materials is one of the sources of their extraordinary properties (high strength, fracture toughness, *etc.*) [1-5]. Further, the reserves of the optimization of composite properties by varying their structures at only microscale level, first of all, volume content and properties of reinforcement are approaching their limits. While some properties (*e.g.*, stiffness) are improved by increasing the volume content of hard reinforcement in composites, other properties (fracture toughness) degrade in this case. To overcome these limits and to design materials with required competing properties, the properties control at several scale levels was suggested (see, *e.g.* [6]).

In his classical paper, Lakes [4] summarized the main ideas of hierarchical material structure as a “basis for synthesizing new microstructures which give rise to enhanced or useful physical properties”. In many works, efforts to create new materials with improved properties on the basis of the hierarchical materials design are described. In the framework of the Japanese “Synergy Ceramics Projects” [6], Kanzaki *et al.* [6] presented an example of an improved material which has both high strength and toughness achieved by combination of aligned anisotropic grains (at microlevel) with the intragranular dispersion of nanoparticles (at nanolevel). Another example of a material with an hierarchical microstructure, and excellent properties (extremely high compressive yield strength) is a “trimodal” Al-composite developed by Ye *et al.* [6].

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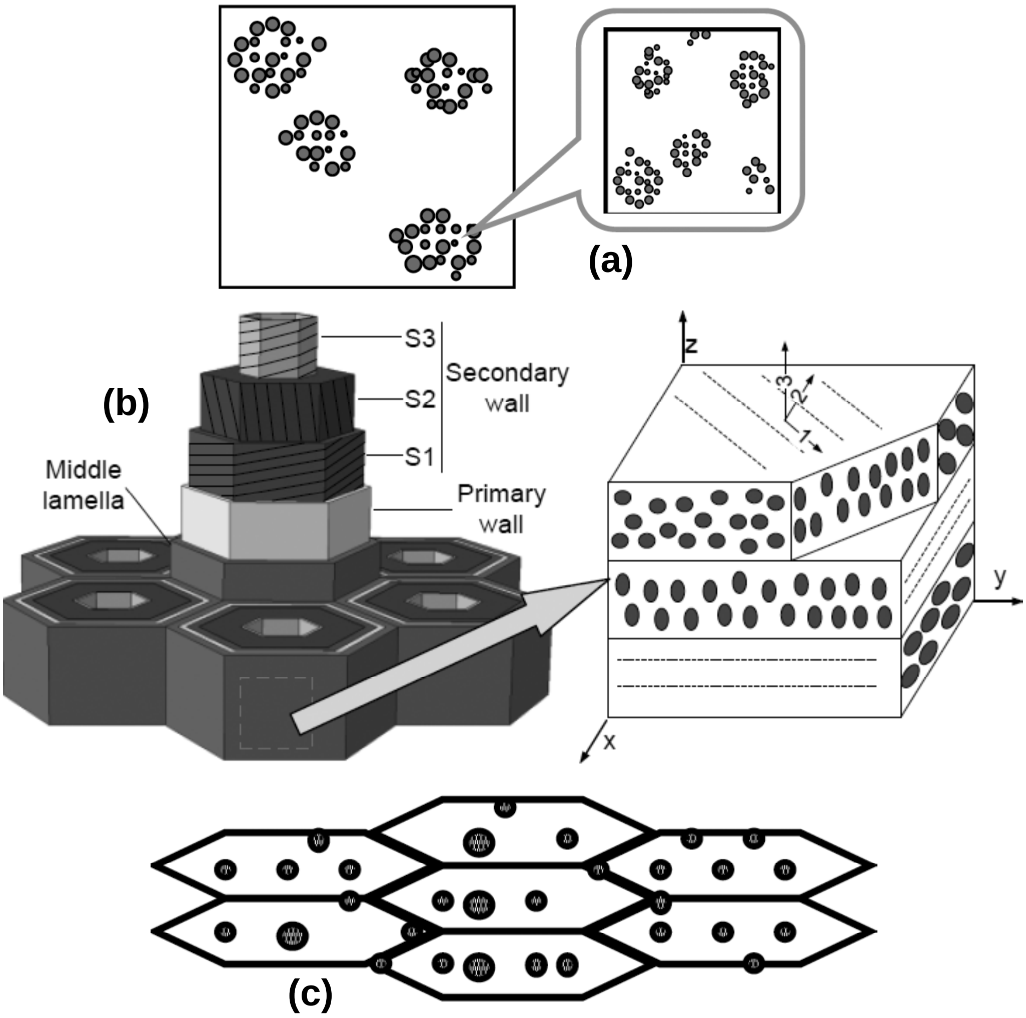

Fig. 1. Schemes: Microstructures of several groups of hierarchical materials: (a) self-similar particle reinforced composites, (b) early wood [84], (c) nanoparticle reinforced ceramics with elongated grains, see [6,5].

Other examples of the successful multiscale design of materials can be listed, among them, the carbon fiber reinforced epoxy/clay nanocomposites, with 85% higher fracture toughness achieved by introducing 4 phr nanoclay in the matrix [8], 30% higher fracture toughness of tool steels achieved by replacing coarse primary carbides by clusters of fine carbides [9], 80% improvement of fracture toughness of carbon fiber reinforced epoxy composites achieved as a result of 0.5 wt.% CNT addition of carbon nanotubes (CNTs) [10], drastic improvements in elastic modulus, compressive strength and interlaminar strength of carbon fiber/polymer composites caused by dispersed carbon nanofibers [12], 30% enhancement of the interlaminar shear strength of woven carbon fabric in epoxy matrix due to the deposition of multi and single walled CNT on fibers [13], 45% increase in shear strength of glass fiber reinforced vinyl ester composite with 0.015 wt.% nanotubes [14], interlaminar toughness improved by 76% and 9% strength improvement in alumina fiber reinforced plastic laminates due to the radially aligned CNTs in both interlaminar and intralaminar regions [11], 80% higher tensile strength in hierarchical Mg matrix reinforced by composite consisting of Al matrix and nanoalumina particles at 0.9%/0.6% reinforcement as compared with monolithic Mg [15].

From these and other investigations in this area, one can conclude that the multiscale composite design, hierarchical structures and tailoring of material properties by controlling structures at different scale levels have a potential to improve different mechanical properties of materials qualitatively.

In order to utilize the potential of multiscale structure design, and to develop the materials with required properties, computational models linking the structures at corresponding scales to the mechanical properties of materials, taking into account the interaction between scales, are necessary.

In this paper, a brief overview of micromechanical models of hierarchical materials, linking the multiscale structures of the materials with their mechanical properties and strength, is given.

2. MICROMECHANICAL MULTISCALE MODELLING OF HIERARCHICAL MATERIALS: AN BRIEF OVERVIEW

In several reviews [1,17,18], the microstructures and sources of unusual mechanical properties of biological materials have been analysed and discussed. In these and other works, some peculiarities of microstructures of these materials have been identified (*e.g.*, multilayer configuration, structural gradients, hierarchical structures), which can be considered as promising recipes for the bioinspired design of industrial materials. In order to transfer these recipes to man-made, industrial materials, with metallic, polymer or ceramic components (instead of proteins or cellulose, *e.g.*), computational, quantitative models are necessary which allow to carry out virtual testing and computational design of hierarchical materials.

A number of mathematical models of hierarchical materials have been developed in the last decades. These models can be grouped according to the materials (and thus typical structures) considered: self-similar particle reinforced composites, bio-and bioinspired materials (bones, nacre, wood, as well materials mimicking these groups), special groups of ceramic, nanoparticle toughened nanocomposites as well as according to the degree of idealization (fractal versus real microstructures) and on "sequential" (with one-sided upper scale-lower scale relationships) and "concurrent" models (with simultaneous upper scale-lower scale or global-local analysis at several levels) [17]. Let us consider some of these groups (see Fig. 1).

<u>Self-similar and multiple reinforced composites.</u> The hierarchical, fractal composite, in which reinforcing elements are recursively composed of matrix and smaller, lower level reinforcements (which are therefore itself composites at a finer scale) were studied in many works. Carpinteri and Paggi [19] used top down approach, the rule of mixture and the generalized Hall-Petch relationship (for hardness), and demonstrated that "a hierarchical material is tougher than its conventional counterpart", and that the material hardness increases with increasing the amount of hierarchy levels. Pugno and Carpinteri [20] employed "quantized fracture mechanics" (an energy-based theory, in which differentials in Griffith's criterion are substituted with finite differences) to analyze a self-similar particle-reinforced composite with fractal-like structure, and derived formulas for fracture energy and failure stress depending on size scales. Joshi and Ramesh [21] used the multiscale secant Mori-Tanaka method (with subscale terms, in particular, grain size, particle size and dispersoid strengthening) to analyze the "trimodal" composites, and computed overall response of the materials. Habibi *et al.* [15] calculated the overall yield strength of hierarchical Mg matrix composites , as a square root of a sum of squared strength contributions from the GND, Hall-Petch and Orowan strengthening. Some groups of hierarchical materials can be considered also as multiple reinforced materials, with reinforcing inclusions of qualitatively different properties and sizes [22]. Gorbatikh *et al.* [23] modeled composites with bimodal size reinforcement (which should represent "two levels of hierarchy") using the rigid inhomogeneities model, and observed that the interaction between hierarchical levels can change the failure mechanism of the material, shifting the potential damage suites from the higher to lower level.

On the basis of the fiber bundle model, Newman and Gabrielov [24] developed the model of hierarchical materials which takes into account the hierarchical microstructural effects not via microstructural description, but via pre-defined hierarchical load sharing rule (HLSR). In the HLSR, the load is localized inside reinforcing elements at each scale level (the reinforcing elements /fibers at each level consist in turn of many elements of lower level). The application of hierarchical load sharing rule is demonstrated on an example in the section 3.2 below.

<u>Nacre.</u> Nacre has been traditionally most apparent and well studied example of biomaterial, whose extraordinary strength is in clear contrast to the brittleness of its components. Among the microstructural peculiarities of nacre, responsible for its unusual properties, the brick and mortar structure, interlocking of platelets, layered configuration, thin organic layers, etc can be mentioned [25]. After the initial period of the experimental-analytical studies of the microstructural sources of nacre strength in 70s-80s [*e.g.*,26], a number of micromechanical models of nacre have been developed in last decade. Among others, one can mention the 3D micromechanical model of nacre with 1000 hexagonal aragonic platelets each surrounded by organic layers in [27], the discrete

lattice model based on continuous damage random threshold fuse network [28], 3D FE unit cell model of nacre (two layers with 150 tablets in each layer) with actual tablet contours obtained from micrographs [29], homogenization model for anisotropic and biomodular mechanical behavior of nacre, based on the BM unit cell in [30], *etc*.

Bone. The microstructures of bones are much more complex than those of nacre. Bone is a porous, cellular materials consisting of multilayered lamellas, built in turn of fibrous layers with different orientations and thicknesses and with various microgeometries for different types of bones (cortical and cancellous). At the nanolevel, the bone is seen as the collagen fibers, surrounded by mineral [31]. Among widely used approaches to the modeling of the microstructure-properties relationships of bones, one can mention:

- multiscale homogenization based models which include typical microstructures at different scale levels. An example of this approach is the multiscale micromechanical model of bones from [32,33], which is based on random homogenization theory and includes bone microstructures via 6 step homogenization procedure (at the scales from 10 nm to 1 mm).
- direct reproduction of complex real microstructures in FE models using high resolution finite element programs. This approach allows to analyze the bone properties at the mesolevel, including the effect of porosity, other microstructural parameters on the mechanical properties and strength of bones. Example of this approach are the voxel-based micro finite element (μFE) model from [34], or works by Niebur *et al.* [35], in which 3D models of bones were rendered from real images.
- nanoscale bone microstructure model, *e.g.* "fractal bone" model (multiple level self-similar composite structure) by Gao [36]. On the basis of this model, Gao demonstrated that a hierarchical material with different properties at different length scales "can be designed to tolerate crack-like flaws". Zuo and Wei [37] analyzed this model with the use of shear-lag approach (as differed with the "tension-shear chain approach" used by Gao) and FEM, and demonstrated that while flaw-insensitivity is still observed in this formulation. Ghanbari and Naghdabadi [38] used the unit cell model with staggered aligned mineral platelets in collagen matrix at the microscale level, for the determination of macro-scale elastic properties of the bone.

Wood and other hierarchical cellular materials. Wood, similarly to bones, represents multiscale, graded, cellular materials with different types of reinforcements at different levels (see Fig. 1b). Hofstetter *et al.* [39-40] developed a micromechanical model based on a three [40] and four-step [39] homogenization schemes for wood. Their approach includes two continuum homogenization steps (random homogenization), and one step based on the unit cell method (periodic homogenization). The elastic properties are determined using the self-consistent scheme and the Mori-Tanaka scheme for the two continuum homogenization steps, respectively. The unit cell method is applied to analyze the assembly of tube-like cellular into the softwood structure. This approach takes into account the microstructure of wood, covering several orders of magnitude, from the cell wall structure, to the structure of fibers, to the macroscopic defects. However, the homogenization method has some limitations when applied to the analysis of damage, and non-linear deformation of wood. Astley and colleagues [41,42] developed multi-scale models and carried out three-dimensional finite element simulations of representative sections of the softwood cell structure. Considering cell walls as 7-layered material, each layer consisting of concentric orthotropic lamellae, they analyzed interrelationships between the macroscopic elastic properties of softwood and the local microstructural characteristics of cells. Further micromechanical models of elastic properties of wood were developed by Bergander and Salmén [43,44] (using the classical lamination theory and semi-empirical Halpin-Tsai equations), Perré [45] (microstructure based FE meshes, homogenisation), and others (see detailed review elsewhere [46]). As different from the homogenization-based models, the discrete multiscale continuum mechanical models make it possible to model damage and strongly nonlinear and time-dependent behaviour of the elements of the wood microstructures.

Analytical models can be used to analyze artificial hierarchical cellular materials, as honeycombs with sandwich walls. So, Fan *et al*. [47] obtained an analytical closed form solution for the strength of hierarchical honeycomb and demonstrated that honeycombs with sandwich walls are much more damage tolerant and stiff than those with solid walls.

Ceramic matrix nanocomposites. According to Sergueeva *et al.* [48], "large majority of so-called nanocomposites developed to date are micro-nanocomposites" (in which grain sizes are in the microscale range, while the inclusions are in the nanoscale) i.e., in fact, hierarchical materials. These micro-nanocomposites includes two of three groups of nanocomposites following the classification by Niihara *et al.* [49] (intra-granular, inter-granular, nano-nano types). Since one of the main mechanism of the nanoreinforcement in these cases is toughening of ceramic matrix, due to additional stresses created by nanoparticles, many models of nanocomposites are based on the fracture mechanics, stress field analysis around the crack/nanoparticles or models of dislocation evolution [51-54]. Awaji *et al.* [53] analyzed the nanoparticle toughening and the residual thermal stresses in intra-type nanocomposites, using a spherical particle inside concentric matrix sphere model, and demonstrated that the thermal expansion coefficients mismatch has a strong effect on the toughening of ceramic nanocomposites.

<u>Hybrid or nanoeingineered fiber reinforced composites.</u> In these composites, additions of small amount of nanoreinforcements (*e.g.*, nanoclay or carbon nanotubes) ensure the strong improvement in the matrix dominated composite properties (like compressive or fatigue strength), additionally to the high stiffness and axial strength provided by strong fibers [56]. Most often, the nanoreinforcements is distributed in the matrix, or grown on the fiber surfaces (or in fiber sizing). While the methods of modeling of mechanical behavior and strength of fiber reinforced composites are well known [55], the main challenges in the modeling of such hierarchical composites lie in the modeling nanoreinforcement clusters and in taking into account the atomistic properties of nanoreinforcement and its interface/ interphase with the matrix. To take into account atomic structure of nanoreinforcement, interphase and polymer matrix in the micromechanical models of nanocomposites, atomistic, molecular mechanics or molecular dynamics based representative equivalent elements models and materials laws are used [57-59]. Multiphase (*e.g.*, 3 phase) models including the matrix, interfacial region, and fillers, or matrix, the exfoliated clay nanolayers and the nanolayer clusters [58,60], as well as the effective particle idealization [62] and the dilute dispersion of clusters models [61] can be employed to take into account both the nanoreinforcement clustering and the interphase effects.

<u>Multiscale computation techniques.</u> The models listed above were developed mainly with the goal to reflect the specific microstructures of given groups of materials. A series of approaches coming "from the other end", namely, multiscale computation techniques, seek to carry out simultaneous upper scale-lower scale or global-local analysis at several levels, and should be applicable ultimately to arbitrary multiscale structures. A lot of scientific efforts were directed at the development of truly multiscale computational techniques, starting from the ***global-local finite element,*** introduced in [63], and other versions of the global-local method (see [64,65]). According to [66], the multiscale computational techniques can be grouped into domain decomposition techniques, multiple scale expansion (homogenization) methods, and superposition based methods. In the framework of the ***domain decomposition techniques***, a macroscale model is decomposed into a series of connected sub-domains, what drastically reduces the the computational costs of the problem solution. In the ***superposition based methods***, the hierarchical decomposition of the solution space into global and local effects is used. Belytschko *et al.* [67] proposed to overlay arbitrary local mesh on the global mesh to enhance the accuracy of solutions of problems with high gradients. Fish [68] developed the s-version of the finite element method, based on the adaptive FEM and error estimation, which idea is to increase the resolution by superimposing an additional, refined local mesh on a coarse global mesh. Several other adaptive versions of FEM have been developed recently: h-version (where convergence is achieved by mesh refinement), p-version (in which the convergence is achieved by increasing polynomial degree), hp-d version (combination of h-and p-extensions in a hierarchical domain decomposition), generalized FEM. A further superposition technique, called "*composite grid method*" was suggested by Fish and colleagues [69,70]. Using the decomposition of a hybrid system into a hierarchical global-local problem and an indefinite local system, they analyzed the deformation of laminated composite shells. In the framework of the *multiscale finite element approach* (called FE2) [71], the microstructure of a material is introduced into the macroscopic models of the material at the level of the Gauss points. The material behavior in each Gauss point of the macroscopic mesh is determined in finer FE simulations. The method is implemented on the basis of interleaved FE algorithms, which constitute a sequence of Newton-Raphson algorithms, and includes local steps on macroscopic and microscopic scales. The simulations are carried out using FETI (domain decomposition) method and parallel computation.

Takano *et al.* [72] developed the finite element mesh superposition technique, which allows to overlay arbitrarily local fine mesh on the global rough mesh. Using this approach, together with the asymptotic homogenization method, Takano and colleagues developed a four level hierarchical FE model of textile composite materials, and carried out the stress analysis in this material. Vernerey *et al.* [73] developed a multiscale micromorphic continuum theory, based on the decomposition of the deformation across scales. In the theory, coupled governing equations representing particular scales are derived.

Still, the multiscale modeling techniques are used currently mainly to analyze mechanical behavior and strength of common composites, not hierarchical materials. Apparently, the numerical challenges related with both complex model design and complex computation techniques still do not allow the efficient analysis of hierarchical materials.

3. EXAMPLES OF HIERARCHICAL MATERIAL MODELS

In this section, we present several examples of the modeling of strength and damage in hierarchical materials. We consider three cases: hierarchical hybrid composites with long fibers and nanoengineered matrix; unidirectional fiber reinforced composites with hierarchically clustered fibers (bundles of bundles of fibers); wood as a gradient, cellular material with layered, composite cell walls. On these examples, one can observe the main areas of applications of different modeling techniques.

3.1. Hybrid composites: UD fiber reinforced composites with nanoeingineered matrix

The development of hybrid composites, with nanoeingineered phases, is a very promising direction to design lightweight materials with improved properties. The fiber reinforced composites with nanoeingineered matrix have much higher strength and fatigue resistance than the neat composites. In order to analyze the effect of the nanoparticle distribution in the matrix and in the interface on the strength of the composites, a computational multiscale model was developed, which includes the fiber/matrix interaction at the higher scale level (microlevel) and nanoclay/epoxy matrix interaction on nanolevel.

On the upper level, the computational unit cell model of the composite consists of cylindrical fibers, surrounded by interphase/sizing layers, and embedded in the matrix. The 3D unit cells with 20 fibers were generated with the use of automatic software Meso3DFiber [74,75]. The material properties and geometric parameters (for the case without nanoparticles) are given in [75]. Fig. 2 shows the unit cell with 20 fibers and interface layers.

The effect of nanoreinforcement (nanoclay) was introduced into the upper level model via the constitutive laws and stress-damage curves obtained from the lower level models. The 3D micromechanical models of a polymer reinforced by nanoclay particles of different shapes were generated with the use of the program code "*Nanocomp3D*" written in ABAQUS Python Development Environment [76]. The unit cells included nanoparticles of different shapes and orientations, surrounded by multilayered effective interfaces. The term "effective interface" means here the interface/interphase layer between the matrix and a particle, reflecting the modified structure of polymer near the nanoparticles. The generalized effective interface model (GEIM), developed in [76] considers the effective interface which consists of several (*e.g.*, two) sublayers, with different properties, typically the stronger layers are outer layers. The effective interface layers (or some of their sublayers) are allowed to overlap, thus, reflecting the fact that the peculiar properties of these regions are caused by modified local atomistic structures, molecular structures or diffusion processes, and do not represent separate phases.

The overlapping of effective interfaces or sublayers of the effective interfaces was realized using Boolean operations in ABAQUS. Fig. 2 shows several examples of the 3D unit cells of nanoclay reinforced epoxy considered in our simulations. The mechanical properties of the phases are given in [76], with the strengths of effective interfaces estimated on the basis of [77]. Using the lower level model, the tensile stress strain curves and stress-damage curves for the different shapes and arrangements of the nanoparticles were determined. These data were used as input parameters (material law) in the upper level model, realized as ABAQUS Subroutine User Defined Field. Several cases were considered: spherical nanoparticles in interface layer and in the matrix, horizontally aligned (i.e., normally to the microscale fiber axes) cylindrical nanoparticles in interface layers, randomly oriented nanoparticles in interface layers and in the matrix, *etc*. In the comparison of hierarchical microstructures with different nanoreinforcement types in the fiber sizing, it was observed that while the horizontal cylinders give several per cents higher stiffness of the nanoreinforced material, they have a lower failure strain than the round nanoparticles. For the microscale model, it means that the availability of nanoreinforcements and its shape and orientation

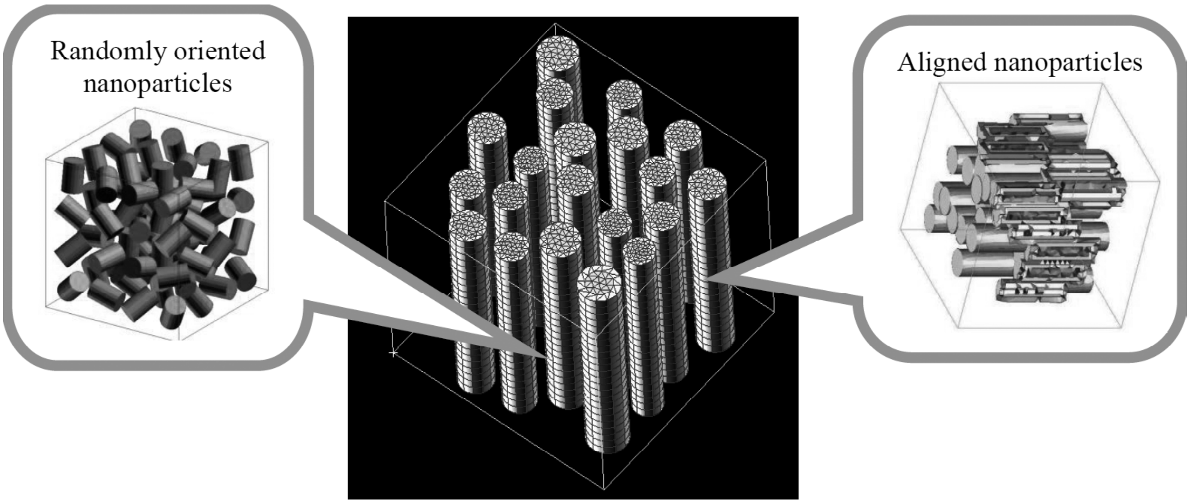

Fig. 2. Micromechanical micro-nanoscale model of fiber reinforced composite with nanoeingineered interfaces. Two examples of lower level models: aligned (horizontal) nanoparticles and randomly oriented nanoparticles, see [76].

can potentially change the overall mechanisms of composite failure: from interface deboding controlled (at horizontal cylindrical nanoparticles) to fiber controlled (at round nanoparticles). Here, an example of relatively simple hierarchical model, which allows to analyze the effect of nanoscale microstructural modifications on the macroscale properties of a materials is shown. This model can be used for the virtual testing and optimization of microstructures of hybrid composites. One could also observe some challenges in using this model: large scale difference in the upper and lower unit cells sizes means numerical difficulties in implementation of load transfer; one-sided upper-lower model linkage and simplified mechanical representation of physical effects (interphases) allow to get only first approximation results. Further computational experiments with this model are under way now.

3.2. Unidirectional fiber reinforced composites with hierarchically clustered fibers: Bundles of bundles and mixed fiber/particle reinforcements

An interesting feature of hierarchical materials is the load transfer between the levels, especially when the microstructure changes (i.e., due to damage or deformation). In order to study the effect of hierarchical structures of composites on their properties, taking into account the peculiarities of load transfer directly, the hierarchical load sharing (HLS) rule can be used [24]. According to this rule, the load is transferred from the upper elements of the hierarchical “tree” (“roots”) to the lower (“branches”) and down to the lowest elements of the material (fibers, in the case of long fiber reinforced composites). The load is shared equally among all the sub-elements of a given branch (as long as they are intact) or among remaining intact sub-elements after some of them fail. In simplest case, this load rule can be directly introduced into the analytical fiber bundle models of composites [5,78,79].

Let us consider a multiscale self-similar composite model (see Fig. 3) subject to a tensile mechanical loading. The composite consists of elements which are either pure matrix or reinforcements at each level. The reinforcing elements at the different levels are self-similar: they, in turn, consist of pure matrix and the lower level reinforcing elements. Since the strain on the fibers and matrix in each element is constant, the load is distributed between the fiber (or strong elements at the given hierarchy level, which represent composites, in turn consisting of fibers and matrix) and matrix proportionally to the Young modulus of a given element [79].

At the lowest level, the strong elements (i.e., fibers) are assigned the strengths according to the Weibull law. If the strength of a given element is less than the applied load, the element (fiber, matrix or bundle) fails and the load is redistributed on the remaining fibers belonging to *the same bundle/ branch*. After all the fibers in the branch fail, the higher level element is considered as failed, and the load is distributed among all the remaining

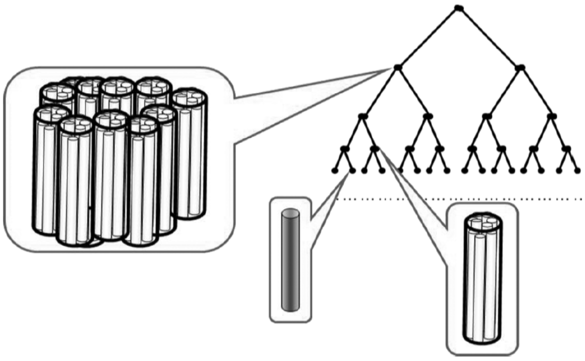

Fig. 3. Hierarchical fiber reinforced composite model, see [79].

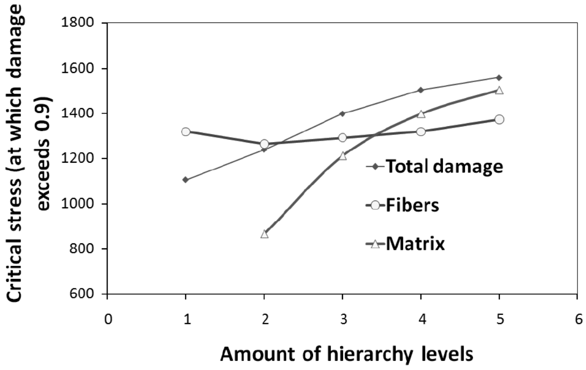

Fig. 4. Critical stress (at which the damage exceeds 0.9) plotted versus the amount of hierarchy levels for glass fiber reinforced composites [79].

elements belonging to the same higher level branch ("bundle of bundles"), and so on.

If the volume content (*vc*) of the reinforcing elements at each level is constant, the global volume content of lowest level fibers in the material is given by $vc_{glob}=vc^{M}$, where *M* – the amount of hierarchy levels. Thus, if we define the total volume content of glass in the composite, the volume content of stronger phase at each scale level is calculated as a M-degree root from this number. Determining the Young modulus of the material at each level using the rule of mixture, we have the Young module at the *j*-th level as [79]:

$$E = vc^{j} + \left(1 - vc\right) E_{M} \left(1 + \sum_{i=1,\, j-1} vc^{i}\right),$$

where E_f, E_M are the Young moduli of (lowest level) fibers and pure matrix respectively, *vc* – volume content of reinforcing elements at each level (assumed to be constant).

Using a program code for the analysis of damage evolution in the multiscale fiber bundle model [79], the effect of hierarchization and structure of the self-similar materials on their damage resistance was investigated. Fig. 4 shows the critical stress (at which the damage in the whole fiber bundle exceeds 0.9) plotted versus the amount of hierarchy levels for the total damage, and separately for fibers and matrix, for glass fiber reinforced composites.

The important observation is that the damage resistance of the multiscale self-similar fiber reinforced composites increases with increasing the amount of hierarchy levels in the material (as differed from the case of "hierarchical tree" considered in [24,79], where increasing the amount of hierarchical levels means reduced damage resistance).

Further, the hierarchical fiber bundle model was generalized to include the case of particulate reinforcement. To do it, the "embedded equivalent fiber" model of particles in a matrix [79] was employed, in which the particle is represented as a cube embedded into the polymer matrix. In the simulations of damage growth in self-similar glass particle reinforced polymer composites, it could be observed that non-hierarchical particle reinforced materials have much higher damage-resistance than hierarchical ones. Still, for the materials with the amount of hierarchy levels 2 and more, the damage resistance increases with increasing the amount of hierarchy levels.

This rather simple model of hierarchical composites allows to analyze the effects of hierarchical structures and hierarchical load transfer in pure form, paying attention only to the hierarchical structures and disregarding the influence of more complex, inhomogeneous structures at each scale level.

3.3. Wood as an hierarchical graded cellular material with multilayered cell walls: Modeling mechanical properties, strength and fatigue life

As different from the idealized self-similar composites, natural hierarchical materials have different structures at different scale levels. As noted above, wood is characterized by layered and gradient structures at the macrolevel, cellular structure at microlevel, with multilayer cell walls, and fiber composite-like structures at the nanolevel. In order to simulate such heterogeneous (over scale levels) structures, complex micromechanical models are required.

In [80-83], the computational model of wood which takes into account the different structural

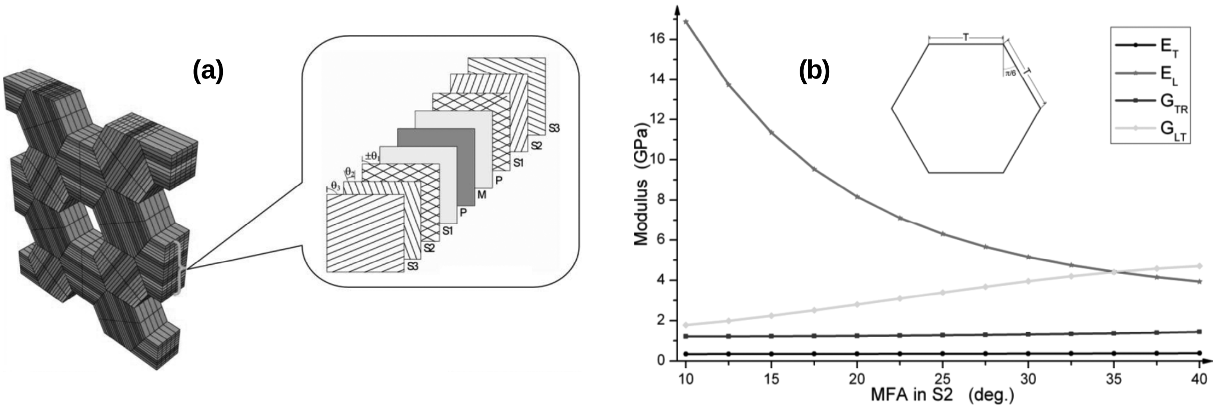

Fig. 5. Example of the FE unit model of earlywood: Honeycomb with multilayered cell walls and various reinforcement inclinations in each sublayer (a) and the effect of microfibril angles in the sublayer S2 on the elastic properties of early wood, see [84,81]. EL and ET the Young's modulus in the longitudinal direction (L) and in the transverse (T) plane, GLT and GTR -shear modulus in LT-plane and in TR(radial)-plane of the wood.

features of the wood at different scale levels, was developed. The model includes four levels of the heterogeneous microstructure of wood:

- Macrolevel: annual rings are modeled as multilayers, using the improved 3D rule-of-mixture,
- Mesolevel: the layered honeycomb-like microstructure of cells is modelled as a 3D unit cell with layered walls. The properties of the layers were taken from the microlevel model,
- Submicro-and microlevel: Each of the layers forming the cell walls was considered as an unidirectional, fibril reinforced composite. Taking into account the experimentally determined microfibril angles and content of cellulose, hemicellulose and lignin in each layer, the elastic properties of the layers were determined with the use of Halpin-Tsai equations

Fig. 5 (left) gives an example of the FE unit model of earlywood. Using the developed model, the effect of microstructural parameters of wood on its deformation behaviour was studied. In particular, the influence of microfibril angle (MFA) and wood density on the deformation behaviour was considered. Fig. 5 (right) shows the influence of microfibril angles (MFA) in the sublayer S2 (broadest and strongest layer in the cell wall) on the elastic properties of the wood. From the computational studies, it was concluded that the variation of microfibril angles represents a rather efficient mechanism of the natural control of stiffness of the main shear load bearing layer of the cell wall. By increasing the MFAs, the drastic increase of shear stiffness in 1-2 direction is achieved, without any sizable losses of the transverse Young modulus and shear modulus in the 23 plane.

In order to analyze the effect of wood microstructure on the fatigue lifetime, the 3D hierarchical model was extended to include the damage process and combined with phenomenological approach toward the fatigue modeling [84]. The progressive damage models for wood were developed, taking into account the strength of the cell wall layer components (lignin, cellulose, polymers) and different strengths of different layers (see [83] for more details). An ABAQUS user subroutine CompFailure.f was developed to describe the failure process of the fibril reinforced cell wall layers, through combining the crack band model and viscous regularization techniques. The damage modelling subroutine provides as output the amount of damaged elements *N* under given loading conditions (i.e., the difference in damage parameters in the material before and after loading).

In order to determine the damage growth rate under cyclic loading, the unit cells (with different initial damage) were subject to the short cyclic tensile strain controlled loading (10 cycles) [84]. (The initial damage can be introduced into the model via a notch, or, alternatively, as random damage). As a result, relationships between between the initial damage level ($D_0(i)$) and damage growth over 10 cycles ($\Delta D(i)/\Delta N$)) was obtained for various hierarchical structures of wood in the form:

$$\frac{\Delta D(i)}{\Delta N} = fD_0(i),$$

where ΔN – amount of loading cycles, here ΔN =10, i – the number of the simulation (in each simulation case, the initial damage level in the model increases,

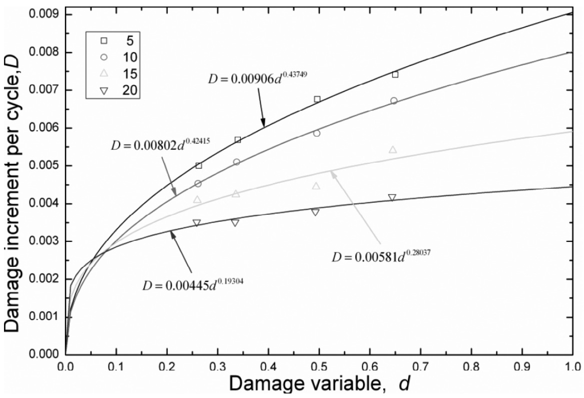

Fig. 6. Fatigue damage accumulation curve (d*D*/d*N* versus *D*) for different microstructures of wood (microfibril angle in the cell wall sublayer S2 varied from 5 o to 20°), calculated using the hierarchical model of wood,see [84]. The formulas give the power approximations of the curves.

from 0 to finally 1), $\Delta D(i)$ – damage growth in *i*-th sequence of ΔN loadings.

Replacing the deltas with differentiating and approximating the relationship between D_o and d*D*/d*N* by a power function, we integrated the formula and determined the lifetime of the material as:

$$N_F = \int \frac{D^{-b}}{a} \mathrm{d}D = \frac{1}{a\left(1-b\right)} G^{1-b},$$

where N_F-lifetime (amount of loading cycles up to the failure). Several unit cells with different pre-damage degrees (i.e., notch lengths) and different microfibril angle degrees (MFAs) in the cell wall layers S2 (largest and strongest layer) were generated and subject to cyclic tensile loading. The curves of fatigue damage accumulation rate plotted versus the damage density (crack length) were approximated by power laws, and the fatigue lifetime was calculated for given microstructures of the materials. Fig. 6 shows the calculated fatigue damage accumulation curve (d*D*/d*N* versus *D*) for different microstructures of wood (microfibril angle in the cell wall sublayer S2, varied from 5 to 20°). The fatigue lifetimes calculated from these curves are given in [84]. Here, hierarchical micromechanical model of wood as a material with various structures and different types of regularity at different scale levels, and its application to the analysis of the microstructure-fatigue lifetime relationships is demonstrated. With such multiscale models, the effects of different microstructural parameters and the synergy between microstructures at different scales can be studied in "virtual experiments". The extension of the hierarchical material model to include the strength and fatigue effects demonstrate the possibilities of the "virtual testing" of hierarchical microstructures.

5. DISCUSSION AND CONCLUSIONS

A short overview of micromechanical models of hierarchical materials (hybrid composites, biomaterials, fractal materials) is given. Several examples of the modeling of strength and damage in hierarchical materials are summarized, among them, 3D FE model of hybrid composites with nanoengineered matrix, hierarchical fiber bundle model of UD composites with hierarchically clustered fibers and 3D multilevel model of wood considered as a gradient, cellular material with layered composite cell walls.

On the basis of the review, the main problems considered in the framework of micromechanics of hierarchical materials can be identified, among them:

(a) Analysis of the load redistribution between reinforcing elements at different scale levels (see *e.g.* [23,79]),

(b) Analysis of possibilities to control different material properties at different scale levels (e.g., if microscale reinforcement ensures high stiffness, while nanoscale reinforcement ensures high toughness, see [6]); Combination and synergy of different strengthening effects at different scale levels (for instance, honeycomb cells in wood at the mesolevel, multilayered cell walls at microlevel, and inclined fibril reinforcements at nanolevel, all ensure the increased stiffness and strength of the wood, using different mechanisms [46,82]),

(c) Effects of nanoreinforcement: using the small scale effects, as dislocations constraints and evolution, peculiarities of nanoparticles (*e.g.*, high strength and very high surface area), to complement the mechanical reinforcing and strengthening effects [2,36,76].

In order to analyze the "pure" hierarchical architecture effects (as clustering or bundles) leading to the load transfer from one scale level microstructure to another, or failure localization in some elements, highly idealized, self-similar, fractal models of materials can be used, *e.g.* fractal composites or hierarchical fiber bundle models [19,20,24,79].

The models based on real multiscale microstructures or their partial idealizations (multiscale homogenization methods, microstructure-based mesh design, …) allow to explore the sources of extraordinary properties of biomaterials (if applied to wood, nacre, bones and other biomaterials), to study the reserves of the material improvement, available in the multiscale tailoring of microstructures, and to analyze the interactions between hierarchical architecture and other microstructural peculiarities of biomaterials (graded structures, cellular and honeycomb-like structures, porosity, brick and mortar structure *etc.*). Further, when applied to man-designed materials (as nanoeingineered hybrid composites), these methods allow to explore the optimal methods of nanoengineering of composites.

For the analysis of the reserves of material improvement related to the nanoscaled reinforcement, the combination of physical (molecular dynamics, atomistics, etc.) and micromechanical models is required.

The main questions determining the future development of micromechanics of hierarchical materials may be summarized as follows:

- What are effects of hierarchical versus non-hierarchical architectures of materials in its pure form (without size effects, microstructure combination effects, nanoeffects, *etc.*) (clustering of reinforcing elements, control of the load transfer, etc.) and in combination with other effects?
- How different elements should be distributed at different scale levels to ensure the best synergy of strengthening effects (on the one side), and the required combination of material responses (*e.g.*, toughness and stiffness), on the other side?
- How to model physical, molecular, atomistic level effects (necessary to study effect of nanoscale reinforcements) in the framework of micromechanics?
- How to develop complex microstructural models of materials with evolving microstructures (*e.g.*, damage) using "concurrent" approaches (with simultaneous upper scale-lower scale or global-local analysis at several levels) rather than "sequential" (with one-sided upper scale-lower scale relationships) models?

Summarizing the above discussion, one can state that a lot of scientific efforts are still required in the micromechanics of hierarchical materials, before these approaches can converge and achieve the level, at which the computational design of materials with optimally tailored multiscale microstructures can be realized.

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REFERENCES

[1] P. Fratzl and R. Weinkamer // *Progress in Materials Science* **52** (2007) 1263.

[2] H. Gao // *Int J Fracture* **138** (2006) 101.

[3] W. W. Schmahl *et al.* // *Mineralogical Magazine* **72** (2008) 541.

[4] R. Lakes // *Nature* **361** (1993) 511.

[5] L. Mishnaevsky Jr., *Computational Mesomechanics of Composites* (Wiley, 2007).

[6] S. Kanzaki, M. Shimada, K. Komeya and A. Tsuge // *Key Engineering Materials* **161-163** (1999) 437.

[7] J. Ye *et al.* // *Scripta Materialia* **53** (2005) 481.

[8] Y. Xu and S.V. Hoa // *Composites Science and Technology* **68** (2008) 854.

[9] H. Berns, A. Melander, D. Weichert, N. Asnafi, C. Broeckmann and A. Groß-Weege // *Computational Materials Science* **11** (1998) 166.

[10] A. Godara *et al.* // *Carbon* **47** (2009) 2914.

[11] S.S. Wicks, R.G. de Villoria and B. L. Wardle // *Composites Science and Technology* **70** (2010) 20.

[12] Y. Iwahori, S. Ishiwata and T. Ishikawa, *Mechanical properties of CFRP using CNF (Carbon Nano-Fiber) dispersed resin*. (Proceedings ICCM-14, San Diego, 2003).

[13] E. Bekyarova, E.T. Thostenson, A. Yu, H. Kim, J. Gao and J. Tang // *Langmuir* **23** (2007) 3970; E. Bekyarova *et al.* // *J Phys Chem C* **111** (2007) 17865.

[14] J. Zhu *et al.* // *Compos Sci Technol* **67** (2007) 1509.

[15] M. K. Habibi, S. P. Joshi and M.Gupta // *Acta Materialia* **58** (2010) 6104.
[16] Y. Dzenis // *Science* **319** (2008) 419.
[17] M.S. Wu // *Materials Science and Engineering: C* doi:10.1016/ j.msec.2010.11.012
[18] M.J. Buehler // *Acta Mechanica Solida Sinica* **23** (2010) 471.
[19] A. Carpinteri and M. Paggi // *Solitons & Fractals* **42** (2009) 2546.
[20] N. Pugno and A. Carpinteri // *Philosophical Magazine Letters*. **88** (2008) 397.
[21] S. P. Joshi and K.T. Ramesh // *Scripta Materialia* **57** (2007) 877.
[22] M.Song, Y.H. He, Z.G. Wu and B.Y. Huang // *Mechanics of Materials* **41** (2009) 622.
[23] L. Gorbatikh, S. V. Lomov and I.Verpoest // *J Mechanics and Physics of Solids* **58** (2010) 735.
[24] W.I. Newman and A.M. Gabrielov // *Int. J. Fracture* **50** (1991) 1.
[25] K.S. Katti and D. R. Katti // *Materials Science and Engineering: C* **26** (2006) 1317.
[26] J.D. Currey // *Proc R Soc Lond* **196** (1977) 443; A.P. Jackson, J.F.V. Vincent and R.M. Turner // *Proc R Soc Lond* **234** (1988) 415.
[27] D.R. Katti, K.S. Katti, J.M. Sopp and M. Sarikaya // *Computational and Theoretical Polymer Science* **11** (2001) 397.
[28] P.K.V.V. Nukala and S. Simunovic // *Biomaterials* **26** (2005) 6087.
[29] F. Barthelat, H. Tang, P.D. Zavattieri, C.-M. Li and H.D. Espinosa // *Journal of the Mechanics and Physics of Solids* **55** (2007) 306.
[30] K. Bertoldi, D. Bigoni, W.J. Drugan // *Composites Science and Technology* **68** (2008) 1363.
[31] J.-Y. Rhoa, In: *Mechanical Properties of Hard Tissues, Encyclopedia of Materials: Science and Technology*, ed. by K. H. Jürgen Buschow *et al*. (Elsevier Ltd.) p. 3723.
[32] A. Fritsch, C.Hellmich and L. Dormieux // *J Theoretical Biology* **260** (2009) 230.
[33] Ch. Hellmich, A. Fritsch and L. Dormieux // *J Biomechanics* **39** (2006) S416.
[34] X. S. Liu, G. Bevill, T. M. Keaveny, P. Sajda and X. E. Guo // *J Biomechanics* **42** (2009) 249.
[35] G.L. Niebur, M.J. Feldstein, J.C. Yuen, T.J. Chen and T.M. Keaveny // *J Biomechanics* **33** (2000) 1575.
[36] H. Yao and H. Gao // *Int J Solids and Structures* **44** (2007) 8177.
[37] S.C. Zuo and Y.Q. Wei // *Acta Mechanica Solida Sinica* **20** (2007) 198.
[38] J. Ghanbari and R. Naghdabadi // *Journal of Biomechanics* **42** (2009) 1560.
[39] K. Hofstetter, C. Hellmich and J. Eberhardsteiner // *Eur. J. Mech. A-Solid* **24** (2005)1030.
[40] K. Hofstetter, C. Hellmich and J. Eberhardsteiner // *Holzforschung* **61** (2007) 343.
[41] R.J. Astley, J.J. Harrington and K.A. Stol // *Ipenz Trans.* **24** (1997) 21.
[42] R.J. Astley, K.A. Stol and J.J. Harrington // *Holz Roh Werkst* **56** (1998) 43.
[43] A. Bergander and L. Salmen // *Holzforschung* **54** (2000) 654.
[44] A. Bergander and L. Salmen // *J. Mater. Sci.* **37** (2002) 151.
[45] P. Perré*, Wood as a multi-scale porous medium: Observation, Experiment, and Modelling, keynote lecture, 1st Inter. Conf. Eur. Society for Wood Mech.* (Lausanne, Switzerland, 2001) 403.
[46] L. Mishnaevsky Jr. and H. Qing // *Computational Materials Science* **44** (2008) 363.
[47] H.L. Fan, F.N. Jin and D.N. Fang // *Composites Science and Technology* **68** (2008) 3380.
[48] A.V. Sergueeva, D.M. Hulbert, N.A. Mara and A.K. Mukherjee // *Frontiers of Nanoscience* **1** (2009) 127.
[49] K. Niihara, A. Nakahira and T. Sekino, In: *Nanophase and previous termNanocompositenext term Materials Symposium*, ed. by S. Komarneni, J.C. Parker and G.J. Thomas (Materials Research Society, 1993).
[50] H. Tan and W. Yang // *Mechanics Materials* **30** (1998) 111.
[51] Z. Zhang and D.L. Chen // *Science and Technology of Advanced Materials* **8** (2007) 5.
[52] S.M. Choi and H. Awaji // *Science and Technology of Advanced Materials* **6** (2005) 2.
[53] H. Awaji, S.M. Choi and E. Yagi // **34** (2002) 411.
[54] M. Sternitzke // *Journal of the European Ceramic Society* **17** (1997) 1061.
[55] L. Mishnaevsky Jr. and P. Brøndsted // *Comput Materials Science* **44** (2009) 1351.
[56] E. Bekyarova *et al*. // *Langmir* **23** (2007) 3970.

[57] L.Y. Jiang, Y. Huang, H. Jiang, G. Ravichandran, H. Gao, K.C. Hwang and B. Li // *J Mechanics and Physics of Solids* **54** (2006) 2436.

[58] M. M. Shokrieh and R. Rafiee // *Computational Materials Science* **50** (2010) 437.

[59] G. M. Odegard, T. S. Gates, K. E. Wise, C. Park and E. J. Siochi // *Composites Science and Technology* **63** (2003) 1671.

[60] J.J. Luo and I.M. Daniel // *Compos Sci Technol* **63** (2003) 1607.

[61] R.G. de Villoria and A. Miravete // *Acta Mater.* **55** (2007) 3025.

[62] N. Sheng, M.C. Boyce, D.M. Parks, G.C. Rutledge, J.I. Abes and R.E. Cohen // *Polymer* **45** (2004) 487.

[63] C.D. Mote Jr. // *International Journal of Num. Meth. Engng*. **3** (1971) 565.

[64] A.K. Noor // *Finite Elements Anal. Design* **2** (1986) 333.

[65] K. M. Maoand and C.T. Sun // *In J Numerical Methods in Engineering* **32** (1991) 29.

[66] K. Haidar, J.F. Dubé and G. Pijaudier-Cabot // *Int J Numerical and Analytical Methods in Geomechanics* **27(13)** (2003) 1187.

[67] T. Belytschko, J. Fish and A. Bayliss // *Computer Methods in Applied Mechanics and Engineering* **81** (1990) 71.

[68] J. Fish // *Computers and Structures* **43** (1992) 539.

[69] J. Fish, V. Belsky and M. Pandheeradi // *Computer Methods in Applied Mechanics and Engineering* **135** (1996) 307.

[70] J. Fish, A. Suvorov and V. Belsky // *Applied Numerical Mathematics* **23** (1997) 241.

[71] F. Feyel and J.L. Chaboche // *Computer Methods in Applied Mechanics and Engineering* **183** (2000) 309.

[72] N. Takano, Y. Uetsuji, Y. Kashiwagi and M. Zako // *Modelling Simul. Mater. Sci. Engineering* **7** (1999) 207.

[73] F. Vernerey, W.K. Liu and B. Moran // *Journal of the Mechanics and Physics of Solids* **55** (2007) 2603.

[74] H. Qing and L. Mishnaevsky Jr. // *Computational Materials Science* **47** (2009) 548.

[75] L. Mishnaevsky Jr. and Povl Brøndsted // *Composites Science and Technology* **69** (2009) 1036.

[76] H.W. Wang, H.W. Zhou, R.D. Peng and L.Mishnaevsky Jr. // *Composites Science and Technology* **71** (2011) 980.

[77] J.K. Chen, G.T. Wang, Z.Z. Yu, Z.P. Huang and Y.W. Mai // *Composites Science and Technology* **70** (2010) 861.

[78] H.E. Daniels // *Proc Royal Society of London* **183** (1945) 405.

[79] L. Mishnaevsky Jr. // *Composites Science and Technology* **71** (2011) 450.

[80] H. Qing and L. Mishnaevsky Jr // *Mechanics of Materials* **41** (2009) 1034.

[81] L. Mishnaevsky Jr *et al*. // *J Wind Engineering* **33** (2009) 183.

[82] H. Qing and L. Mishnaevsky Jr // *International Journal of Solids and Structures* **47** (2010) 1253.

[83] H. Qing and L. Mishnaevsky Jr // *Computational Materials Science* **50** (2010) 479.

[84] H. Qing and L. Mishnaevsky Jr // *Computational Materials Science* **50** (2011) 1644.